

DIALOG

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DN: cn=/LDR/,
c=US
Date: 2008.06.28
14:36:23 -04'00'

Set	Items	Description
S1	44080	S SIMULAT? (3N) ANNEAL?
S2	10489	S GLOBAL (2N) MINIMUM
S3	262400	S POTENTIAL (3N) ENERGY
S4	338602	S MOLECULAR (2N) DYNAMICS
S5	29	S S1 AND S2 AND S3 AND S4
S6	25	RD S5 (unique items)
S7	2997	S DOCK? (S) SUBSTRATE (S) ENZYME
S8	0	S S6 AND S7
S9	313	S S4 AND S7
S10	135	RD S9 (unique items)
S11	16423486	S MODEL? OR SIMULAT?
S12	117	S S10 AND S11
S13	234014	S P450
S14	13	S S12 AND S13
S15	58136	S FORCE (2N) FIELD
S16	249187	S POTENTIAL (2N) ENERGY
S17	15433	S DISTANCE (5N) (FIX? OR CONSTRAIN?)
S18	24	S S15 AND S16 AND S17
S19	11	RD S18 (unique items)

? show files

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